NIKE3D Code Maintenance and Enhancement

Michael A. Puso
(925) 422-8198
puso1@llnl.gov

The objective of this work is to enhance, maintain, and support the implicit structural mechanics finite element code NIKE3D. This tool is LLNL's primary capability for simulating the slowly evolving or steady-state response of nonlinear solids and structures. New features are continually added to accommodate engineering analysis needs. Maintenance includes bug fixes and code porting to new or updated platforms. User support includes assisting analysts in model debugging and general analysis recommendations.

Project Goals

Code enhancement requires continuous interactions with users as well as new features to meet our evolving needs. Each year some activities are pre-planned, *e.g.,* completing production versions of higher-order elements and nodally integrated tetrahedrals. Other efforts arise in response to real-time needs. Such "just in time" enhancements included new material model capabilities for weapons analysts and new contact analysis features.

Relevance to LLNL Mission

Structural analysis is one of the most important functions of Engineering and motivates in-house maintenance for LLNL's suite of codes. NIKE3D, in particular, is a premier code for handling difficult nonlinear static structural analysis problems. It has the most diverse and robust contact algorithms at the Laboratory to handle the complex interactions of unbonded material interfaces.

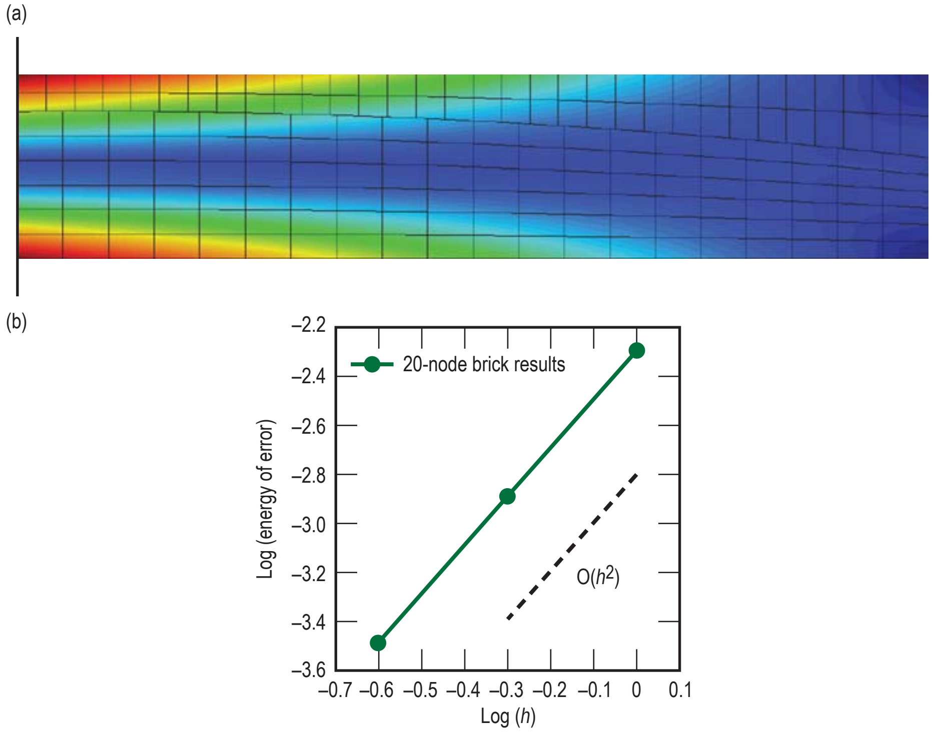
FY2007 Accomplishments and Results

A number of new element technologies and discretization technologies have been developed at LLNL, most notable being higher-order elements (10-node tetrahedrals, 20- and 27-node hexahedrals), nodally integrated tetrahedrals, and meshless methods. Efforts are required to make them fully integrated functionalities available for production use by analysts. For example, these implementations exploited more modern, hierarchical data structures available in Fortran 95.

NIKE3D's existing technique of writing a monolithic restart database did not work with these new features. Instead, the data needed to be written and read recursively to perform this task for each data structure. The process of writing these dedicated recursive algorithms was automated using a PERL script adapted from one first created by the Diablo project and then adapted for new data structures in DYNA3D.

To finalize the production capability of higher-order elements, modifications were made for using GRIZ to visualize higher-order element results. Previously,

Figure 1. (a) Bending stress shown on 20-node model of loaded cantiliever beam with (curved) contact surface separating top and bottom. (b) Convergence plot demonstrating optimal quadratic convergence of the energy norm of the discretization error.



higher-order elements results could be visualized only by GID. Now TrueGrid and Cubit can be used to build quadratic element meshes, and our quadratic mortar contact algorithms can be used without loss of quadratic convergence rate (Fig. 1) for nonlinear analysis using higher-order elements (Fig. 2) in NIKE3D.

New material model features were added in support of weapons analysis. One example is a new thermal-plastic model that captures thermal material response over an arbitrary range of temperatures (Fig. 3). Finally, a number of contact features were added. Most notably, new work has begun on the improvement of the quasi-Newton contact solver. The quasi-Newton method is used for solving the nonlinear system of equations in NIKE3D and is a keystone to its success. Nonetheless, there is much room for improvement. As part of this effort, a new Armijo-type line search algorithm was added along with several small modifications to improve solution robustness.

Related References

1. Puso, M. A., and T. A. Laursen, "A Segment-To-Segment Mortar Contact Method for Quadratic Elements and Large Deformations," *Computer Methods in Applied Mechanics and Engineering,* in press.
2. Christensen, P. W., *et al.*, "Formulation and Comparison of Algorithms for Frictional Contact Problems," *International Journal for Numerical Methods in Engineering,* **42**, pp. 145-173, 1998.

FY2008 Proposed Work

Our existing mortar contact implementation currently uses an N^2 search algorithm. In FY2008, we will implement better and faster search algorithms such as the bucket sort.

We will implement an improved quasi-Newton method. A number of new methods have been created in the area of optimization that could be converted to treat computational contact mechanics.

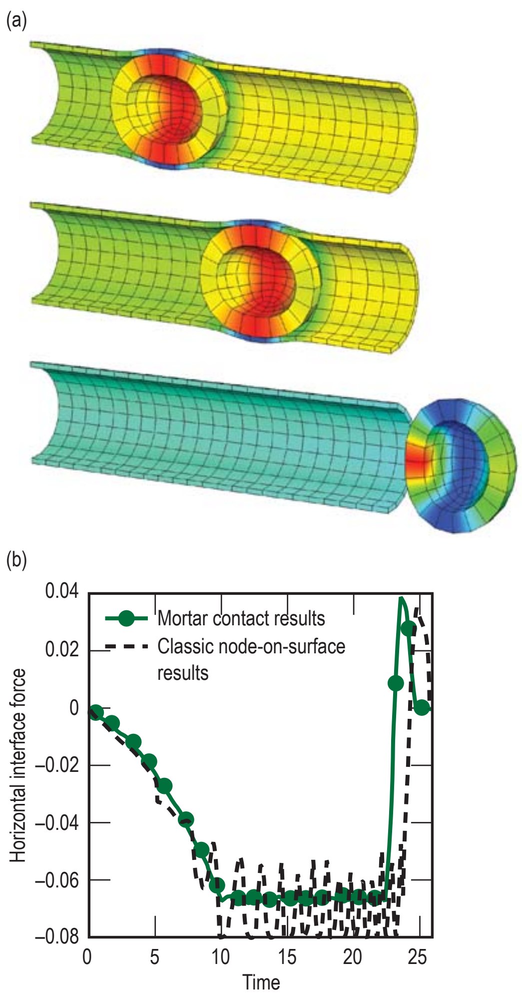


Figure 2. (a) Simulation of elastic sphere being forced out of pressurized elastic tube. Twenty-node brick elements are used. (b) Horizontal force on tube versus time. This force is mainly due to frictional resistance. Force is very smooth for mortar contact results, whereas node-on-surface force is not.

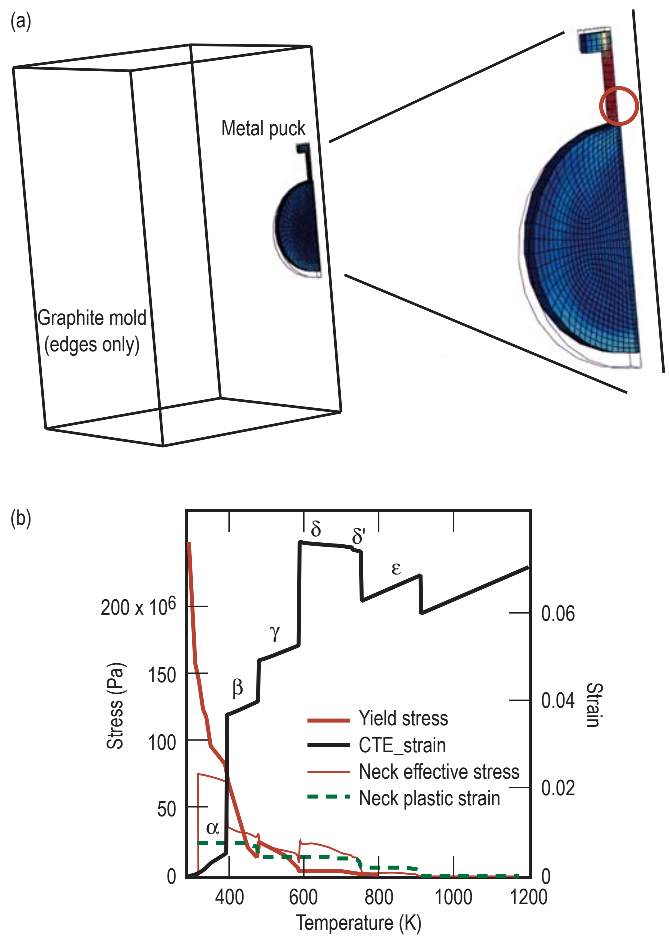


Figure 3. (a) Metal "puck" cast inside graphite mold (3-D solid mesh not shown). (b) Evolution of stress and strain at critical location (red circle in (a)) in casting as metal is cooled. The thermal phase changes indicated in yield stress and CTE strain are provided in the arbitrary format of the new material model feature.